2-(N-methylanilino)-6-(5-nonyl) pyrazine

Inchi: InChI=1S/C20H29N3/c1-4-6-11-17(12-7-5-2)19-15-21-16-20(22-19)23(3)18-13-9-8-10-14

InchiKey: OHQIPGUAYZNHIR-UHFFFAOYSA-N

Formula: C20H29N3

SMILES: CCCCC(CCCC)c1cncc(N(C)c2ccccc2)n1

Mol. weight [g/mol]: 311.46

CAS: 116660-11-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	5.708		Crippen Method
mcvol	275.080	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660118&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume